6. CAMx INPUT DATA PREPARATION

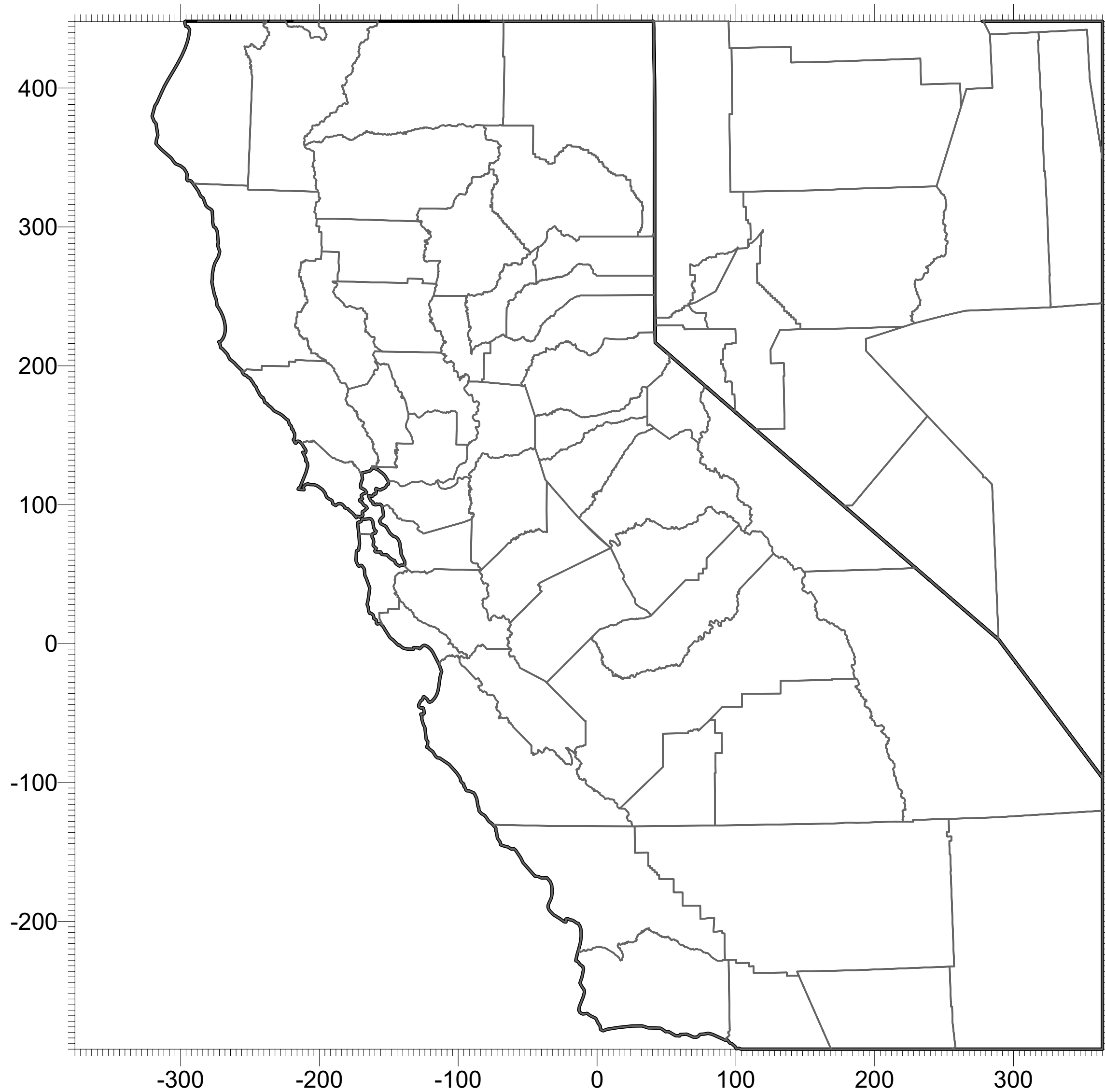
Several data preparation tasks are required to provide CAMx with various inputs that define the meteorology, emissions, initial and boundary conditions, surface characteristics, and photochemical conditions of the atmosphere. The bulk of work associated with meteorology and emissions is described in previous sections. However, some additional processing is needed for these components just before the air quality model is run. This section begins with a discussion on the air quality modeling grid specification; it is critical to define the grid system extent and resolution before the development of most of the CAMx input fields can begin. This section then goes on to describe the procedures to develop and/or format the various input files for CAMx, and finally lists the model options that were invoked in the base and diagnostic simulations.

CAMx DOMAIN AND GRID SPECIFICATIONS

The spatial domain (or volume) on which Eulerian models operate is defined as a three-dimensional grid, which is used to discretize the environment into averages contained within many relatively small grid cell volumes. The modeling grid should be defined with sufficient size and resolution to capture all of the significant physical processes and transport patterns that affect pollutant concentrations in the focus area. Obviously a balance must be struck between grid size and resolution, both because of resource constraints (computing power), and because of limitations inherent in all Eulerian models to characterize physical phenomena at small scales (<1 km horizontally).

Therefore, an important step in the design of an ozone modeling system is specifying the extent of the domain and resolution of the grid. The air quality modeling domain and grid specifications for this study were based on CARB's meteorological, emissions and air quality modeling configuration for CCOS. The CARB is currently undertaking simulations of the July/August 2000 CCOS and July 1999 ancillary episodes using CAMx applied on a very large regional domain on a Lambert Conic Conformal projection with 4-km grid spacing (Figure 6-1). The MM5 model was operated by CARB, NOAA, and BAAQMD directly on the projection shown in Figure 6-1, but on a slightly larger extent (190 by 190 grid points – a similar grid was used to develop gridded emission inputs using EMS-95). The MM5CAMx interface processor provided the link that basically passed through the MM5 output variable fields to CAMx without the need for projection mapping and horizontal interpolation.

The RAMS model used earlier in this study operates on a Rotated Polar Stereographic projection, and so the RAMSCAMx interface processor provided the link that performs the necessary manipulations of the RAMS output to properly feed into CAMx on the CCOS Lambert projection. As described in Section 4, the definition of the RAMS polar grid was carefully coordinated to match the CCOS/CAMx Lambert projection as closely as possible in the area of greatest concern (central California). Initial CAMx simulations using RAMS meteorology were applied on a domain similar to Figure 6-1, but using 12-km cell size and employing a nested 4-km grid over the Bay Area, Sacramento, northern San Joaquin Valley, and the Monterey Bay Area (see modeling protocol prepared by ENVIRON et al., 2002). With the desire to better align the BAAQMD modeling with CARB and other districts, this nested grid arrangement was abandoned midway through the project.



CCOS 185x185 4km Domain
LCP Center: (120.5W, 37N)
Standard Parallels: 30N, 60N
Coordinates: (-376,-292) to (364,448)

Figure 6-1. The coverage of the CARB/CCOS air quality modeling domain. Grid spacing over the entire region is 4 km. Map projection is Lambert Conformal.

In some CAMx sensitivity tests, a high-resolution nest was specified to cover the urbanized portion of the immediate SFBA. The grid cell resolution was 1 km (for use with RAMS meteorology) and 1.33 km (for use with MM5 meteorology developed by BAAQMD). Since topography is a major factor in ozone formation in the SFBA, a 4-km grid likely does not resolve certain wind flow features that have proven critical to the accurate placement and formation of ozone. These initial tests were undertaken with 4-km emissions but with the higher resolved meteorological inputs fields (referred to in CAMx as "flexi-nesting", as the model allows for the user to provide any, all, or none of the needed fields for each nested grid). As described in

Sections 6 and 7, RAMS, MM5, and CAMx tests with the high resolution nest did not definitively show improved results in the meteorological and ozone concentration fields, but additional testing is warranted and will be carried out in follow-on modeling work. Gridded emission estimates (area, on-road, biogenics, etc.) may need to be reprocessed to the higher resolution using new spatial surrogates if we are to investigate the full potential effects of this fine grid. Point sources would not need to be reprocessed as those inputs are not dependent upon model resolution.

In the vertical, CAMx operates in a terrain-following coordinate system, and can match the layer structure of any meteorological model providing three-dimensional gridded input fields. In this project, three basic meteorological configurations were used, all with different vertical grid structures: the ATMET RAMS modeling for both episodes, the NOAA/BAAQMD MM5 modeling for July/August 2000, and the CARB/BAAQMD modeling for July 1999. CAMx was configured for each of these three different layer structures depending upon on which source of meteorological data was used to drive the photochemical model, and which group developed the configuration. In all cases, CAMx layers were set to span several meteorological layers up to the respective CAMx model tops. Allowing air quality model layers to span multiple meteorological models above the boundary layer depth is a common practice to conserve memory requirements without degrading performance, and in this particular project the technique was particularly important given the very large horizontal grid structure. Early tests were conducted with CAMx using RAMS meteorology to test the effect of different layer aggregation schemes and model top altitudes; there was little sensitivity to both.

The specific grid structures are summarized below, along with the group responsible for developing the configuration:

- <u>RAMS meteorology</u>: CAMx resolved the atmosphere into 24 layers up to ~7.5 km above the surface (ENVIRON/BAAQMD protocol);

- <u>MM5 meteorology for July/August 2000</u>: CAMx resolved the atmosphere into 20 layers up to ~15 km above the surface (UCR);

- <u>MM5 meteorology for July 1999</u>: CAMx resolved the atmosphere into 16 layers up to ~4.5 km above the surface (CARB).

EMISSIONS PROCESSING

While EMS-95 generates hourly, speciated, gridded emission files for use in air quality models, there are some final steps to perform before CAMx can use them. EMS-95 provides separate elevated point (anthropogenic and fire sources) and gridded surface (biogenic, area, and on-road mobile) emission files in ASCII text formats. Processing of these files was accomplished using readily available and standard pre-processing software tools.

The first step was to convert the low-level gridded files to the UAM binary format required by CAMx. Then these files were "windowed" from the large 4-km emissions grid (190 by 190 grid cells) to the slightly smaller air quality modeling grid (185 by 185 grid cells). Finally, these files were "merged" into a single all-encompassing gridded emissions input file for CAMx. This last step also shifted the emissions ~1 km eastward and southward to improve the alignment between the emissions grid with the meteorological and air quality grids[1].

The first step in processing the elevated point source files was to generate a common list of sources over all days of the modeling episode (day-specific point emissions were provided for all fire sources and certain major anthropogenic sources). This placed all anthropogenic source at the top of the list, and all fire sources at the end. Second, the anthropogenic and fire sources were merged together into a single file for each day, using the common list developed in step one. Third, large elevated NOx point sources were selected for the CAMx Plume-in-Grid (PiG) treatment based on a minimum threshold daily NOx emissions rate of 1 ton/day. During this process, the program sorts the PiG sources from all days to generate a unique list of ranked sources. Finally, a program was run that reads the list of PiG sources, flags them in the file for treatment, and generates a single binary model-ready file for each day containing all elevated point sources.

Note that these emission files were developed by CARB in Pacific Daylight Time (PDT). This required CAMx to be run in PDT as well, and for either the CAMx output to be converted to Standard Time, or for the air quality observations to be converted to PDT, in the model performance evaluation.

For the July/August 2000 episode, the CARB provided day-specific emissions for all components (area, point, on-road, biogenic), except for July 28 (one of two model “spin-up” days). For that date, gridded emissions were linked to August 1 (both weekdays with similar temperatures). Point sources for July 28 were assigned from August 1 (anthropogenic) and July 31 (fires).

For July 1999, the CARB provided day-specific emissions for biogenics and on-road mobile sources. Area and point sources were provided for a representative weekday and weekend day (July 4 and 5, respectively). These were linked to specific weekend days and weekdays for over the modeling period (July 8-12).

METEOROLOGICAL PROCESSING

Raw output from the meteorological models needs to be converted to formats and variables used by CAMx specifically. ENVIRON has authored widely used RAMS and MM5 translation software to complete this task. The software includes the ability to interpolate data from the native map projections used by the meteorological models to any projection to be specified for air quality model (CAMx may be applied on Lambert Conformal, Polar Stereographic, or UTM projections, or in geodetic latitude/longitude). These programs also convert meteorological fields from UTC to PDT time zones.

CAMx requires meteorological input data for the parameters described in Table 6-1. All of these input data were derived from the RAMS and MM5 simulation results. RAMS output fields were translated to CAMx-ready inputs using the RAMSCAMx translation program, while MM5

[1] The CARB developed their emissions grid as closely as possible to the CCOS Lambert modeling grid, but was never able to exactly match the spherical assumptions used in MM5 and CAMx in their GIS processing of spatial surrogates.

output fields were translated using the MM5CAMx program. Both of these programs perform several similar functions:

1. Extract data from the meteorological grids to the corresponding CAMx grids; in this study, the extraction includes a mass-weighted interpolation from the RAMS polar stereographic grid to the CAMx Lambert grid, with appropriate rotation of wind variables (no projection interpolation was necessary for MM5 meteorology).

2. Perform mass-weighted vertical aggregation of data for CAMx layers that span multiple meteorological model layers.

3. Diagnose key variables that are not directly output by MM5 or RAMS (e.g., vertical diffusion coefficients and cloud information).

Table 6-1. CAMx meteorological input data requirements.

CAMx Input Parameter	Description
Layer interface height (m)	3-D gridded time-varying layer heights for the start and end of each hour
Winds (m/s)	3-D gridded wind vectors (u,v) for the start and end of each hour
Temperature (K)	3-D gridded temperature and 2-D gridded surface temperature for the start and end of each hour
Pressure (mb)	3-D gridded pressure for the start and end of each hour
Vertical Diffusivity (m^2/s)	3-D gridded vertical exchange coefficients for each hour
Water Vapor (ppm)	3-D gridded water vapor mixing ratio for each hour
Cloud Cover and Rain	3-D gridded cloud opacity and liquid water content for each hour

Both programs have been written to carefully preserve the consistency of the predicted wind, temperature and pressure fields output by the meteorological models. This is the key to preparing mass-consistent inputs for CAMx, and therefore for obtaining high quality performance from CAMx.

Vertical diffusivities (Kv) are an important input to the CAMx simulation since they determine the rate and depth of mixing in the planetary boundary layer (PBL) and above. RAMS provides direct output of Kv and turbulent energy, while MM5 provides output of either PBL depth or turbulent energy (depending on the user’s selection of PBL model) but not Kv. Therefore, RAMS provides a choice of either using Kv directly or diagnosing Kv from turbulent energy. However, the use of MM5 absolutely requires that Kv be diagnosed from available output.

In general, our experience has been that diffusivities from meteorological models require careful examination before they are used in air quality modeling. This may be because the air quality model results are much more sensitive to diffusivities than the meteorological model results. In the case of RAMS, our evaluations suggested that the diagnosis of Kv from turbulent energy within the RAMSCAMx interface program was better behaved, both from a conceptual and magnitude basis, than the direct pass-through of RAMS Kv. For MM5, the diagnosis of Kv within the MM5CAMx interface program was based on the profile approach of O’Brien (1970), which depends upon PBL depth output by MM5. Numerous sensitivity tests were undertaken early in the project to test various Kv input fields. Given the very poor model performance achieved in early CAMx simulations, these tests were not conclusive. Additional such tests will be necessary in follow-on work.

DEVELOPMENT OF ANCILLARY INPUTS

The preparation of ancillary input files include initial/boundary conditions, land use distribution, chemistry parameters, albedo/haze/ozone fields, and photolysis rates.

Initial and Boundary Conditions

The initial conditions (ICs) are the pollutant concentrations specified throughout the modeling domain at the start of the simulation. Boundary conditions (BCs) are the pollutant concentrations specified at the perimeter of the modeling domain. One of the reasons for performing regional scale modeling rather than urban scale modeling is to minimize the importance of ICs and BCs. Using a large regional domain moves the boundaries far away (in distance and transport time) from the study area. Including several "spin-up" days prior to the episode period allows time for the influence of initial conditions to be removed.

The developmental history of IC/BC inputs for CAMx is complicated, as each group undertaking CAMx modeling for the July/August 2000 CCOS episode has developed their own unique set of inputs. A concerted effort to unify these inputs among the groups is warranted and should be undertaken in follow-on work. The approach detailed here describes the CB-IV inputs developed by ENVIRON for the July/August 2000 episode. A single consistent set of inputs were also developed by CARB for the July/August 2000 and July 1999 episodes, and these have been adopted for use by the BAAQMD for the July 1999 episode. The BAAQMD also developed IC/BC inputs for the SAPRC99 chemical mechanism.

July/August 2000 CCOS Episode

The very first CAMx simulations for the July/August 2000 episode were carried out by the University of Riverside (UCR) in 2002 as CARB's modeling contractor. UCR modeling was based on the NOAA MM5 simulations at the time, and thus IC/BC inputs were needed for the 24 layer structure through 15 km (as described above). UCR adopted IC/BC values developed for the SARMAP program, which included separate vertical profiles of ozone, NOx, VOC, and CO for over land and over water areas of the grid. No attempt was made to modify the concentration profiles based on the CCOS observational dataset as it was not yet available at the time. UCR reported satisfactory ozone results in the Bay Area and Sacramento regions using CAMx with these IC/BC inputs.

However, it quickly became apparent to the BAAQMD modelers that high ozone levels measured at the surface and aloft in central California during the July/August 2000 episode were likely augmented by the very many large regional fires throughout the western U.S., particularly in Southern California, Oregon, and Nevada. Therefore, ENVIRON developed revised IC/BC inputs, based on the UCR profiles as a starting point (Table 6-2), to reflect the role of regional

Table 6-2. UCR SARMAP-based ozone profiles (ppm) by CAMx layer.

Height (m)	West O3	North/South/East O3
23.76	0.025	0.04
49.17	0.0258	0.0415
104.69	0.0266	0.0432
168.11	0.028	0.0469
240.29	0.0295	0.051
369.98	0.0315	0.0551
526.48	0.0348	0.0624
703.77	0.0385	0.07
903.86	0.0427	0.07
1128.67	0.0455	0.07
1386.98	0.0475	0.0698
1733.35	0.0493	0.0692
2207.02	0.0511	0.0683
2853.89	0.0531	0.0669
3751.15	0.0546	0.0654
5131.22	0.0566	0.0634
7277.25	0.06	0.06

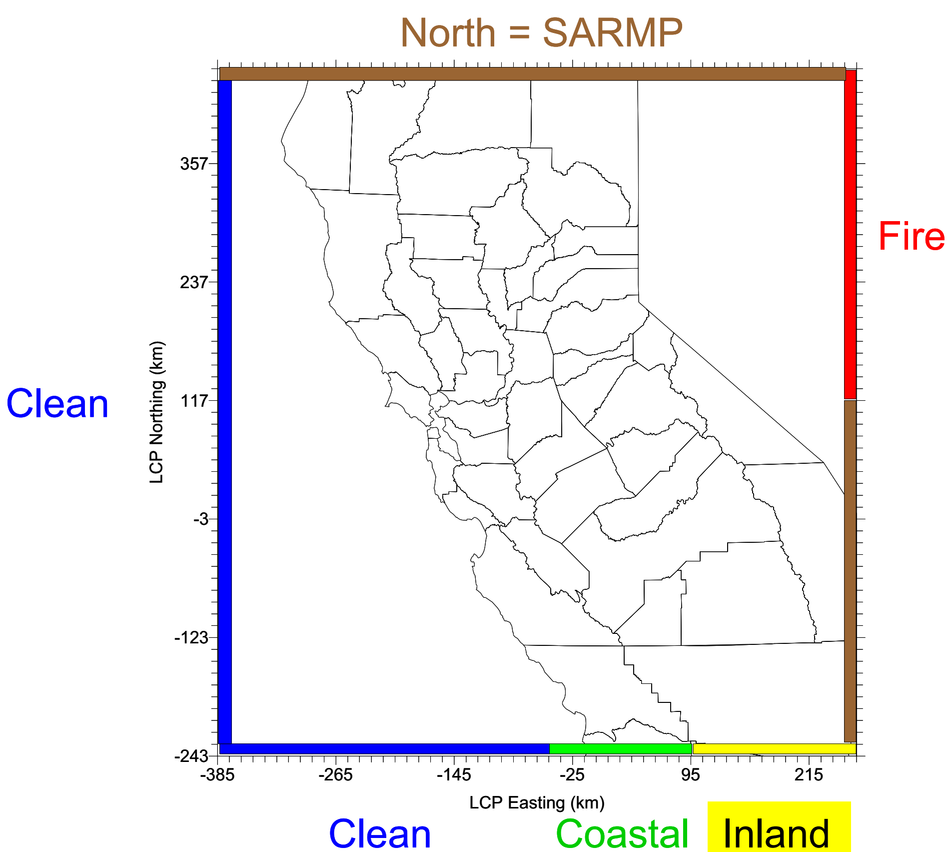


Figure 6-2. Scheme to assign various CAMx domain boundary segments for regional influences.

fires on elevated layers of NOx, VOC, CO, and ozone particularly on the southern, eastern, and northern boundaries. Additional analyses of surface ozone and NOx observations, ozonesondes, aircraft data, satellite pictures, and back trajectories were conducted to support the revision. The CAMx boundary was divided into separate segments to reflect varying regional influences (Figure 6-2).

Ozone

The SARMAP-based ozone profiles were in pretty good agreement with aircraft and ozonesonde observations. These ozone profiles were used as-is along the west, north, and east boundaries. The southern boundary was split into three parts: clean, coastal, and inland.

The clean section spanned the westernmost cells over the ocean; SARMAP western boundary ozone was applied to this area. The coastal section was based on hourly surface ozone observations from Santa Barbara County (Lompoc, Santa Ynez, and Paradise) during the July-August, 2000 episode. The average diurnal profile over these sites and over all days of the episode (Figure 6-3) was applied to all layers within the lowest 1 kilometer. Above 1 km, the SARMAP southern boundary ozone profile was used. Inland, the episode-average diurnal profile from Lancaster (Figure 6-2) was applied to all layers within the lowest 2 km. Again, SARMAP southern boundary ozone was used aloft.

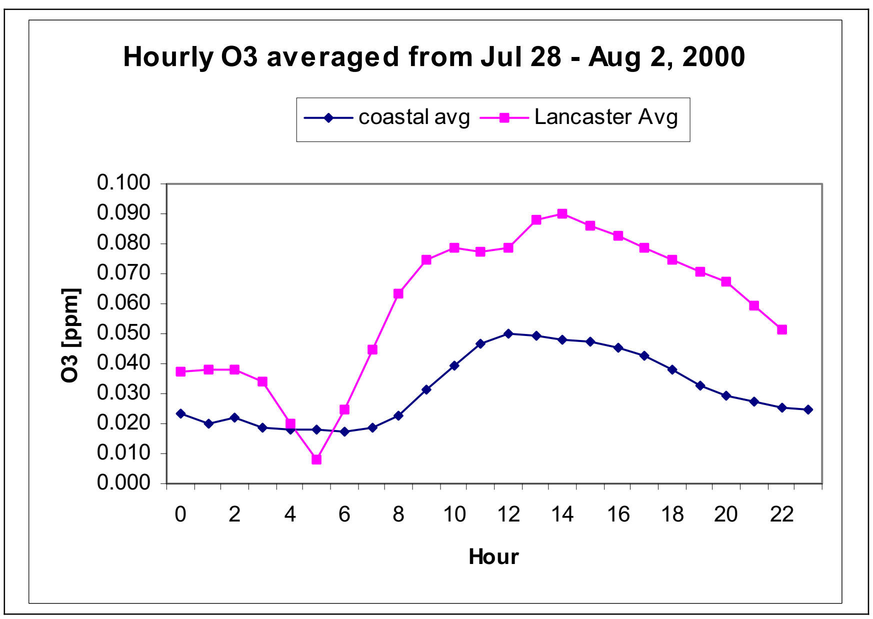


Figure 6-3. Episode-mean diurnal ozone profiles at Lancaster and for the average over all sites in Santa Barbara County (coastal average).

NOx

NOx was set at 0.04 ppb NO and 1 ppb NO2 over the lowest 1 km of the western boundary and over the lowest 1 km of the “clean” section of the southern boundary, based on aircraft observations over the ocean on July 30, 2000. Above 1 km, the SARMAP NOx profile was applied in both areas. SARMAP decreased both species by about two orders of magnitude from 1 to 7 km.

Along the coastal and inland sections of the southern boundary, NO and NO2 were set to 0.5 ppb and 3.5 ppb, respectively, based on mean NOx measurements near and along this boundary. These values were held constant over the lowest 1 km at the coast and 2 km inland. Above these levels, NO and NO2 were held constant at 0.25 ppb and 1.25 ppb (the SARMAP surface values), respectively, to take the Pechanga fire into account. Based on winds aloft during the episode, smoke from this rather large fire east of Los Angeles was likely transported north and northwest toward the southern boundary of the model.

Along the southern half of the eastern boundary, and along the entire northern boundary, SARMAP NOx profiles were used: NO and NO2 were constant at 0.25 ppb and 1.25 ppb, respectively, through the lowest 1 km, and then dropped about 2 orders of magnitude by 7 km. Along the northern half of the eastern boundary, NO and NO2 were also set at 0.25 ppb and 1.25 ppb, respectively, within the lowest 3 km; but SARMAP NOx concentrations were doubled aloft to account for the numerous wildfires in Nevada.

CO

Carbon monoxide was based on SARMAP in most areas as it was held constant at 200 ppb except near the top of the domain, where it decreased 20% along the west, north, clean section of the south, and southern half of the east boundaries. CO was doubled aloft over the northern half of the eastern boundary to account for fire influences.

VOC

The SARMAP-based VOC profile is constant at 34.6 ppbC through the lowest 1 kilometer and then decreases by two orders of magnitude approaching 7 km. The UCR boundary conditions use this profile for all four boundaries. Individual UCR/SARMAP VOC species concentrations near the surface are shown in the table below.

Table 6-3. SARMAP VOC Concentrations in the lowest 1 km (ppb).

PAR	20.500
OLE	0.414
ETH	0.702
TOL	0.246
XYL	0.135
ISOP	0.050
FORM	5.780
ALD2	1.520

For our revised boundary conditions, the SARMAP VOC profile was used on the north boundary and southern half of the east boundary. VOCs along the west boundary and clean section of the south boundary were reduced by a factor of 3 within the lowest 1 kilometer, but retained the standard SARMAP-based VOC values aloft. On the coastal and inland portions of the south boundary, VOC species were held constant at 34.6 ppbC in all layers to ~7 km to account for fire plumes from southern California. On the northern half of the east boundary, 34.6 ppbC was set through the lowest 3 km; aloft, SARMAP VOCs were doubled to account for the wildfires burning in Nevada.

Top Boundary Conditions

The UCR SARMAP-based lateral boundary conditions for the east/north/south boundaries at ~7.5 km were used to set top boundary conditions for ozone, NOx, CO, and VOCs for the RAMS-based vertical grid structure. The UCR top concentration files were used directly for the MM5-based vertical grid structure.

Initial Conditions

The initial condition file was split into a “clean” section and “dirty” section (Figure 6-4). The clean section, represented by the gray area in the figure below, covers the ocean and Bay Area. The “dirty” area, spanning northern California, Nevada, and the San Joaquin Valley, covers areas where wildfire emissions were predominant. These were applied to both RAMS-based and MM5-based CAMx modeling grids. Since these initial conditions were dispersed during the simulation spin-up days, this step-like arbitrary distribution did not influence the simulation on key episode days.

In the clean section, UCR SARMAP-based vertical profiles of CO, VOC, NOx, and western boundary ozone were used. In the dirty section, the north/south/east SARMAP ozone boundary profile was selected. CO, NOx, and VOC were assumed to be two times the SARMAP-based boundary layer concentrations in all layers to account for the previous buildup of forest fire smoke as of July 28 and 29.

<u>Development of IC/BC Inputs for BAAQMD SAPRC99 Applications</u>

Boundary conditions for organic compounds were interpolated from aircraft measurements conducted during the CCOS 2000 field campaign. Aircraft measurements provided vertical profiles of 40 VOC model species in the SAPRC99 chemical mechanism as implemented in CAMx version 4.03. These model species are HCHO, CCHO, RCHO, ACET, MEK, PROD, RNO3, PAN, PAN2, BALD, PBZN, PHEN, CRES, NPHE, GLY, MGLY, METH, MVK, MEOH, HC2H, CO2H, RC2H, CH4, ETHE, ISOP, TERP, MBUT, MTBE, ETOH, NROG, LOST, ALK1, ALK2, ALK3, ALK4, ALK5, ARO1, ARO2, OLE1, and OLE2.

For each model layer, all available aircraft measurements were averaged to obtain the boundary conditions. When there was no measurement in a layer, boundary conditions were generated from values in the layers above and below through linear interpolation. For model layers above the maximum flight altitude (~1.6 km), values at the maximum flight height were used for the boundary conditions. A sensitivity test was conducted to reduce the boundary values for HCHO, CCHO, and RCHO to one third of the observations. It was shown that the resulting change in

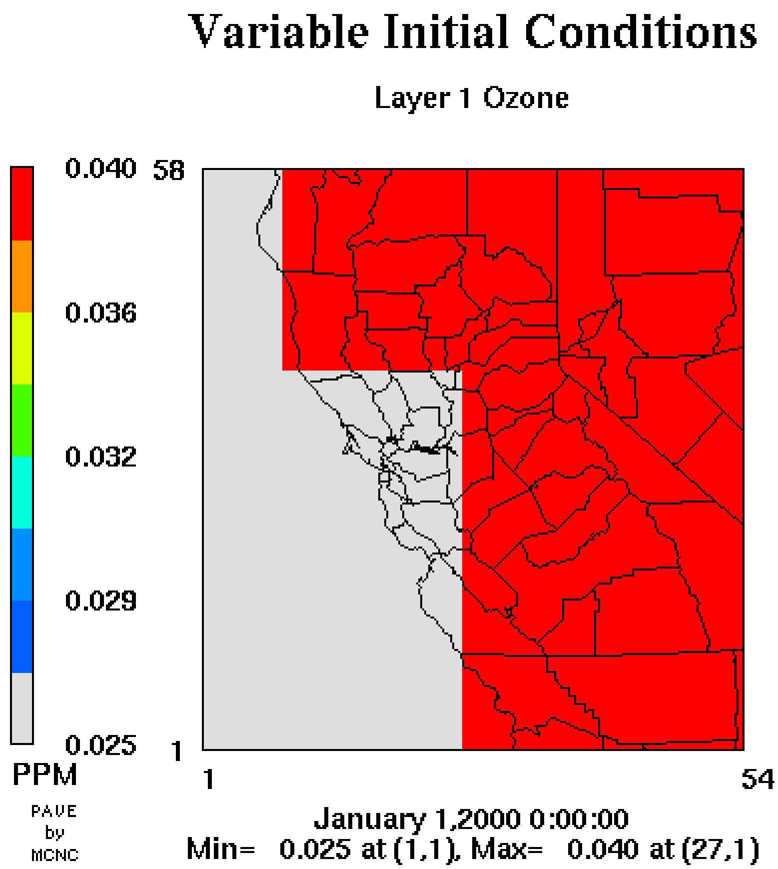


Figure 6-4. Distribution of "clean" and "dirty" zones for the assignment of initial conditions for the July/August 2000 episode. Shown is the RAMS-based CAMx modeling grid, but the same pattern was applied to the MM5-based CAMx grid.

peak ozone was negligible (~1 ppb). The lower values for HCHO, CCHO, and RCHO were adopted to minimize the effect of boundary conditions on ozone formation in the model domain.

Boundary conditions for inorganic compounds were based on synthesis of previous studies. Boundary values for O3 range from 25 ppb at the surface to 75 ppb near the tropopause, resembling vertical profiles from ozonesonde data over the ocean. Boundary values for NOx were specified to range from 1.5 ppb at surface to 0.2 ppt at the tropopause, and that for CO from 200 ppb at the surface to 110 ppb in the top layer of the model. Boundary values for N2O5, NO3, HONO, HNO4, and H2O2 were set to range from 10 ppt at the surface to 0.001 ppt at the tropopause. Other model species were set to be virtually zero at the boundary.

Top boundary conditions were set to equal to the boundary values in the top layer of the model, and initial conditions in each layer were set to be the same as corresponding boundary values described above.

July 1999 Episode

The CB-IV initial and boundary condition inputs for this episode were obtained from the CARB. The CARB simply copied the profiles of NOx, VOC, CO, and ozone directly from their CAMx simulations of the July/August 2000 episode, which included a top boundary condition for ozone of 70 ppb, and moderate levels of NOx and VOC on the lateral boundaries based on several past studies, including the 1990 SARMAP and southern California modeling applications dating back to the late 1980's. The top boundary conditions for ozone in particular were set by CARB to reflect the high ozone measured by ozonesondes in the central valley during the fire-influenced July-August 2000 episode. This may be too high for the July 1999 episode since very little fire activity was present. Besides their consideration of ozonesonde profiles, the CARB did not analyze CCOS aircraft data to support their selection of lateral boundary conditions.

Evaluation of Initial/Boundary Conditions on SFBA Ozone

The potential influences of initial and boundary conditions were evaluated in this project. Inert runs were conducted using the RAMS/CAMx modeling system to show the flow from the boundaries into the domain and it's subsequent dispersion across California. The sensitivity to initial and boundary conditions on ozone formation in central California was evaluated using the Direct Decoupled Method (DDM) of sensitivity coefficients (one of the CAMx Probing Tools). This test was undertaken for the July 1999 episode using the MM5/CAMx modeling system, and is discussed further in Section 7.

Both inert and DDM analyses clearly showed that the initial conditions are only somewhat dispersed and removed from the simulation during the spin-up days prior to the core episode days, and that the northern boundary contributes significantly to background concentrations entering the SFBA. This is in contrast to original thinking, which assumed that the western boundary was the key contributor in defining background levels entering the Bay Area. But as seen in Figure 6-5, the flow from the northern boundary heads south along the California coastline and is brought into the SFBA via the sea breeze circulation. Near-surface flow from the western boundary heads southeast in parallel with the California coastline, and is hardly mixed into the on-shore flow. Therefore, the selection of boundary conditions for the northern boundary is much more crucial to the CAMx simulation than for the western boundary. In fact, modeling evidence suggests that CCOS aircraft measurements off the California coast are measuring aged smoke plumes from Oregon or recirculated air from central California, and so are not appropriate for setting western boundary conditions.

Surface Characteristics (Landuse)

CAMx requires gridded landuse data to characterize surface boundary conditions, such as roughness, deposition parameters, albedo, vegetative distribution, and water/land boundaries. The land cover categories utilized by CAMx are based on the 11 category system established in RADM, which are parallel with SAQM.

Land use inputs were developed by several entities, depending on the modeling configuration employed. At the start of the project, ENVIRON developed landuse inputs from a USGS national 30-second land cover database for use with the 12/4-km nested RAMS/CAMx modeling configuration. UCR developed landuse inputs for the MM5/CAMx modeling configuration as part of their modeling of the July/August 2000 episode. That dataset was directly generated from the MM5 land use fields. The BAAQMD adopted that landuse file for subsequent MM5/CAMx modeling of the CCOS episode. For the July 1999 episode, the CARB adopted the UCR inputs

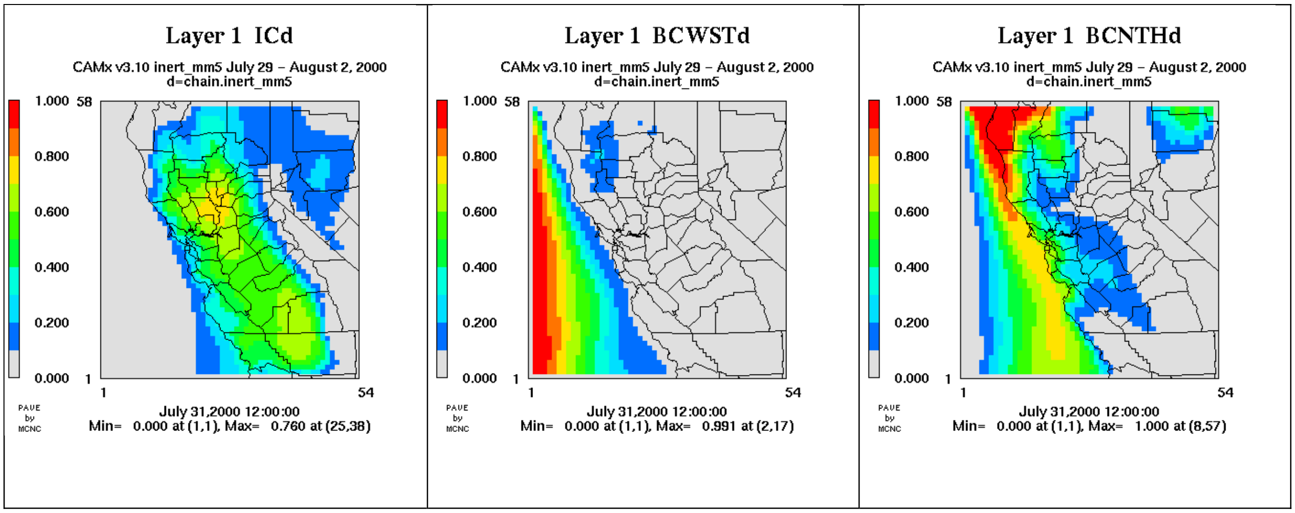


Figure 6-5. Relative contributions at the surface from initial (IC), western BC (BCWST) and northern BC (BCNTH) in the RAMS/CAMx grid system from an inert tracer simulation.

directly from their CCOS modeling. The BAAQMD directly used the CARB landuse file for MM5/CAMx modeling of the July 1999 episode.

Chemistry Data

Three input files define the chemistry used in CAMx.

Chemistry Parameters: The chemistry parameters file selects which chemical mechanism to use and specifies the rate constants for the thermochemical reactions. CAMx was run with two different mechanisms. All developmental and sensitivity runs employed the most up-to-date version of the Carbon Bond 4 mechanism (CB4), which is referred to as “mechanism 3” in CAMx. Mechanism 3 is the CB4 mechanism with updated (circa 1995) radical termination reactions and isoprene chemistry as used for the OTAG modeling of the eastern U.S. CAMx was also run with the SAPRC99 mechanism, referred to as “mechanism 5” in CAMx. SAPRC99 is newer, provides up-to-date reaction rates, and the hydrocarbon lumping scheme resolves VOC more precisely. Generally, it has performed similarly to CB4, although it tends to produce somewhat higher (~5-10 ppb) ozone in NOx-rich conditions such as highly urban environments. SAPRC99 contains many more reactions and species than CB4, and this leads to model run times are nearly twice that of CB4. Therefore, SAPRC99 was used for modeling after final model configurations were set according to developmental simulations.

Photolysis Rates: The photolysis rates file determines the rates for chemical reactions in the mechanism that are driven by sunlight. The photolysis rates file was prepared using version 4 of the TUV radiative transfer model developed at NCAR. The rates file is essentially a very large multi-dimensional lookup table that defines the variation of photolysis reactions over zenith angle, altitude, surface UV albedo, haze turbidity, and total vertically integrated ozone column density.

Albedo/Haze/Ozone File: This file specifies how these three photolysis-related parameters vary in time and space for the CAMx simulation. The photolysis rates and albedo/haze/ozone files must be coordinated to function together correctly. The surface albedo was calculated based on the gridded landuse data. The stratospheric ozone column data were based on available satellite data from http://www.cpc.ncep.noaa.gov. Since there was no source of regionally specific haze data for the study area, constant haze turbidity representative of rural areas was assumed over the entire grid. Tests with CAMx over a wide but representative range of turbidity values have shown that model results are not particularly sensitive to how this parameter is set. ENVIRON developed the albedo/haze/ozone file for the RAMS/CAMx configuration, while UCR and BAAQMD developed this file for the MM5/CAMx configurations used in the July/August 2000 and July 1999 episodes.

CAMx MODEL OPTIONS

CAMx has several user-selectable options that are specified for each simulation through the CAMx control file. Most of these options follow naturally from other choices about model inputs. There are three additional optional inputs that were selected for this project: the advection scheme, the plume-in-grid scheme and the chemistry solver. See the CAMx User's Guide (ENVIRON, 2003) for more details on these options. The selection for each option was determined at the early stages of base case model development.

Advection scheme: CAMx has two optional methods for calculating horizontal advection (the movement of pollutants due to horizontal winds) called Bott and Piecewise Parabolic Method (PPM). These schemes are relatively new and exhibit little artificial ("numerical") diffusion. Our experience with these schemes suggests that PPM is a better overall approach given that Bott tends to generate some small but definite numerical artifacts. Hence, we selected the PPM scheme for this study. On the other hand, the CAMx Decoupled Direct Method (DDM) probing tool is coded to only utilize the Bott approach. Therefore, simulations with DDM required the use of Bott.

Plume-in-Grid: CAMx includes an optional sub-grid scale plume model that can be used to represent the dispersion and chemistry of major NOx point source plumes close to the source. This technique was developed primarily to better treat the chemistry of very large NOx plumes (such as coal-fired EGUs) in VOC-rich environments such as experienced in the Midwest U.S. We conducted some early tests with the PiG invoked, but the "major" NOx sources in California are relatively weak, and so there was very little sensitivity to the PiG. Therefore, while the major NOx sources were flagged for PiG in the point source input files, the algorithm was not invoked when CAMx was run.

Chemistry Solver: CAMx provides two options for the numerical solution scheme for the gas phase chemistry. The first option is the CMC fast solver that has been used in every prior version of CAMx. The second option is an IEH solver. The CMC solver is fast and more accurate than most chemistry solvers used in current ozone models. The IEH solver is even more accurate than the CMC solver but significantly slower. The CMC solver was used for this study since it is faster and it leads to very little difference in ozone concentrations.